NANOMATERIALREGISTRY

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RTI International

Workshop on A Uniform Description System for Nanomaterials

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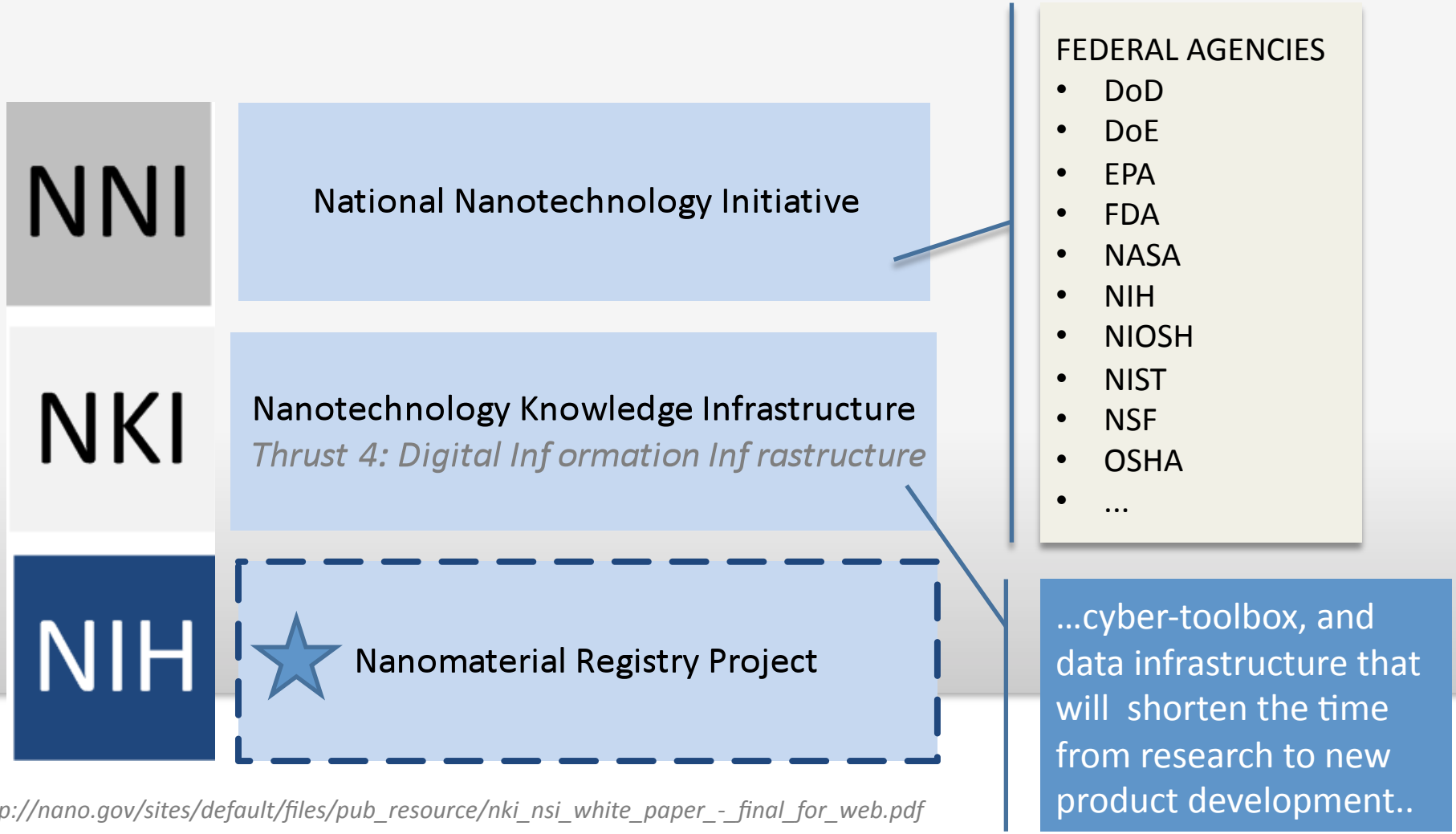
FEDERAL NANOTECHNOLOGY INITIATIVE

The NNI Coordinates R&D in nanoscale science, engineering, and technology



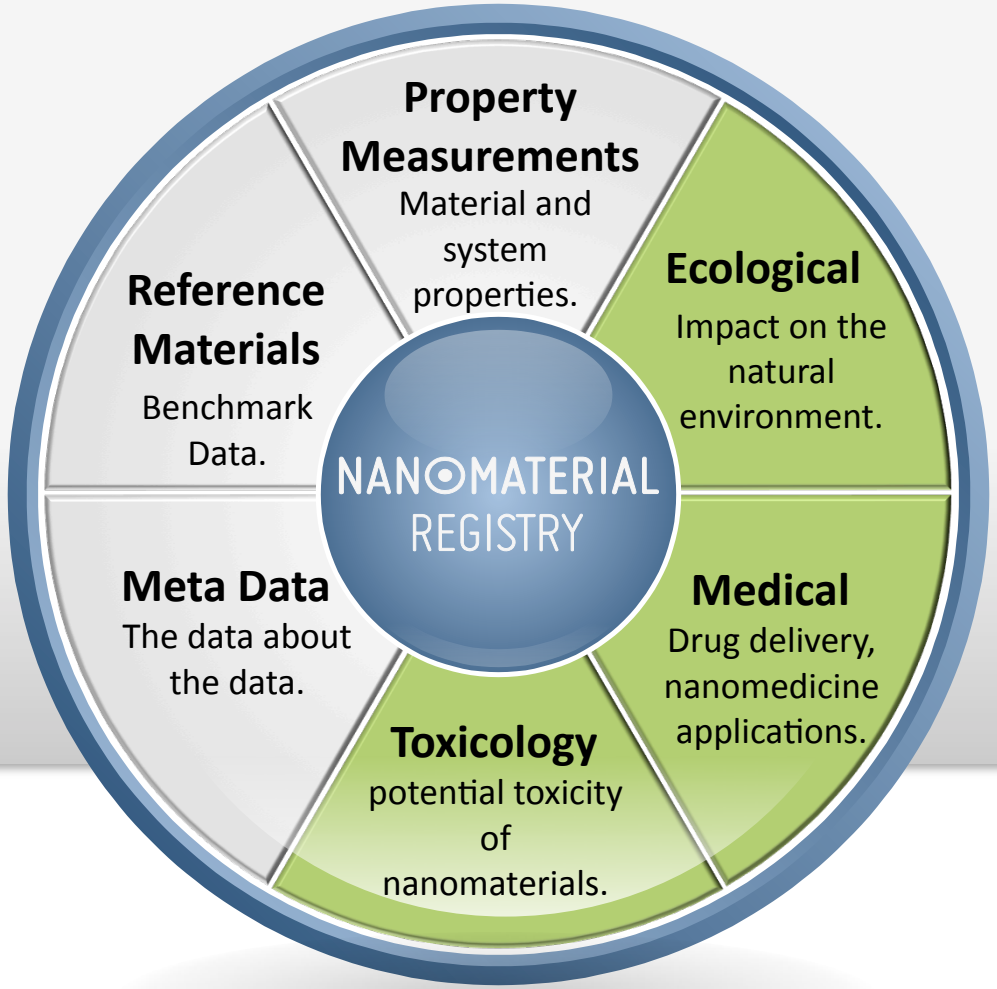
http://nano.gov/sites/default/files/pub_resource/nki_nsi_white_paper_-_final_for_web.pdf

NANOMATERIALREGISTRY

What you can expect to find in the Nanomaterial Registry

DATA DOMAIN

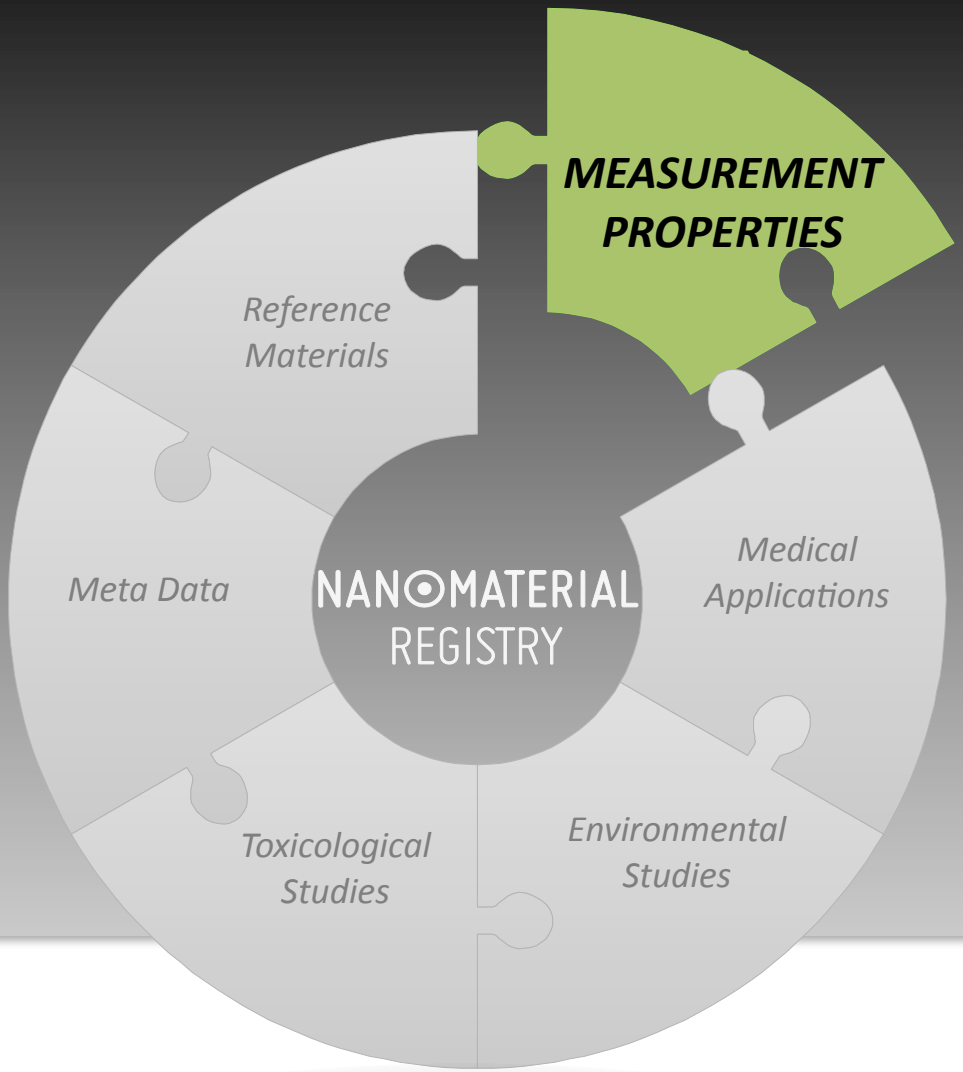
DOMAIN: CHARACTERIZATION + STUDY DATA



- **Validated** both programmatically and by a team of scientists
- **Integrated** through controlled vocabulary and data formatting
- **Relevant** growing body of data that is available to the public

NANOMATERIALREGISTRY

LOOKING ACROSS THE CHARACTERIZATION DATA



- Particle Size
- Size distribution
- Surface area
- Shape
- Composition
- Aggregation/ Agglomeration state
- Purity
- Surface chemistry
- Surface charge
- Surface reactivity
- Solubility
- Stability

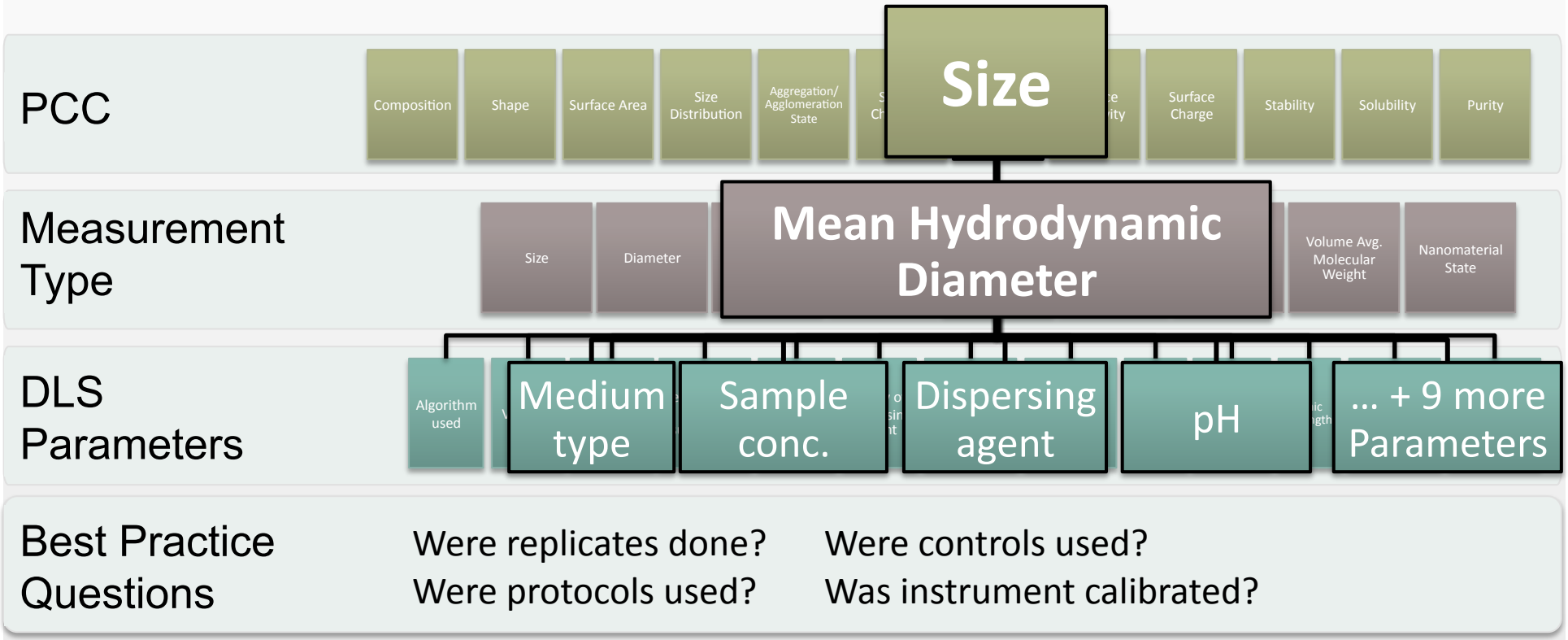
PCC Data — *12 Physical and Chemical Characteristics*

Protocal & Parameters — *Information about instrumentation settings*

Best Practice Questions — *Meta data about measurement technique*

A **controlled vocabulary** of PCC & measurands have been identified (https://www.nanomaterialregistry.com/resources/**Glossary**.aspx)

Minimal Information About Nanomaterials



NANOMATERIALREGISTRY

DATA RECORDS IN THE REGISTRY

PDF (TEXT)

PEER REVIEWED LITERATURE

ORIGINAL RESEARCH PUBLICATION

Nanomedicine (Lond). 2012 Aug;7(8):1197-209. doi: 10.2217/nnm.12.18. Epub 2012 May 14.

Silver nanoparticles do not influence stem cell differentiation but cause minimal toxicity

Samberg ME, Loboa EG, Oldenburg SJ, Monteiro-Riviere NA.

DATA IS CURATED INTO THE DATABASE

PARSED DATA

NANOMATERIAL REGISTRY

TWO UNIQUE DATA RECORDS

NR1130, NR1131

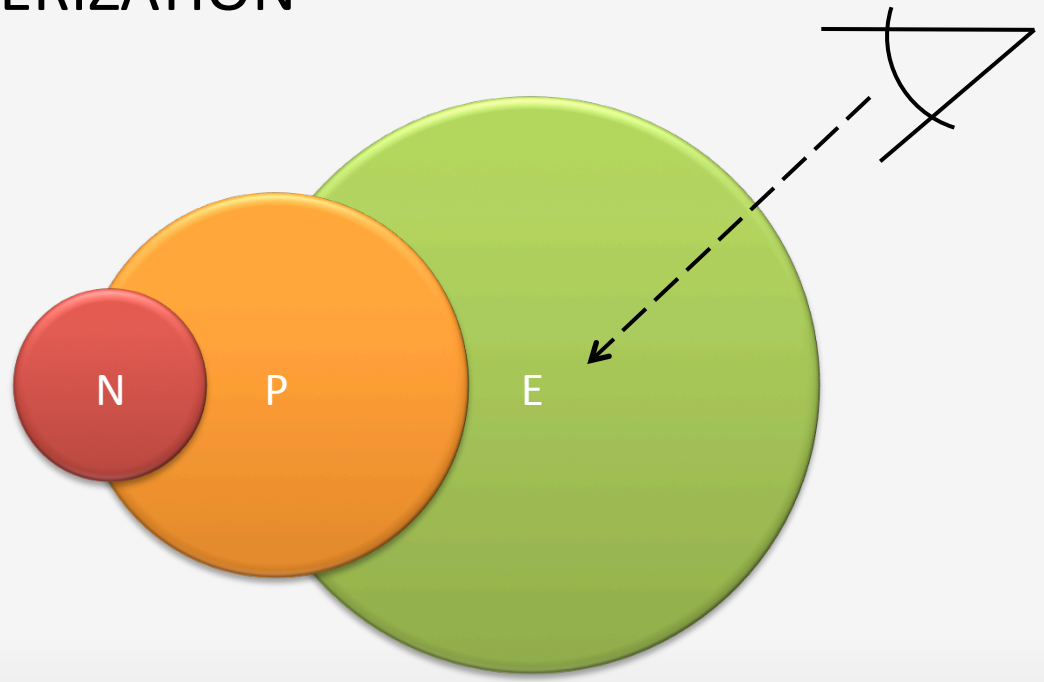
- MULTIPLE COMPOSITIONS? No
- MULTIPLE SIZES? Yes: 10 nm, 20 nm
- MULTIPLE MANUFACTURERS? No

FROM JOURNAL TEXT: *"….Two solutions of spherical Ag-NPs were obtained from NanoComposix (CA, USA), each at Ag-NP concentration of 1.00 mg/ml with diameters of 10 and 20 nm….."*

NANOMATERIAL CHARACTERIZATION

Individual nanoparticles exist in

- POPULATION (P) of particles
- ENVIRONMENT (E)



Observed Characteristic = $f(P,E)$

Additional considerations:

- Individual Particle
- Population/sampling
- Environment
- Time
- Measurement technique

$= f(P,E,T,M\ldots)$

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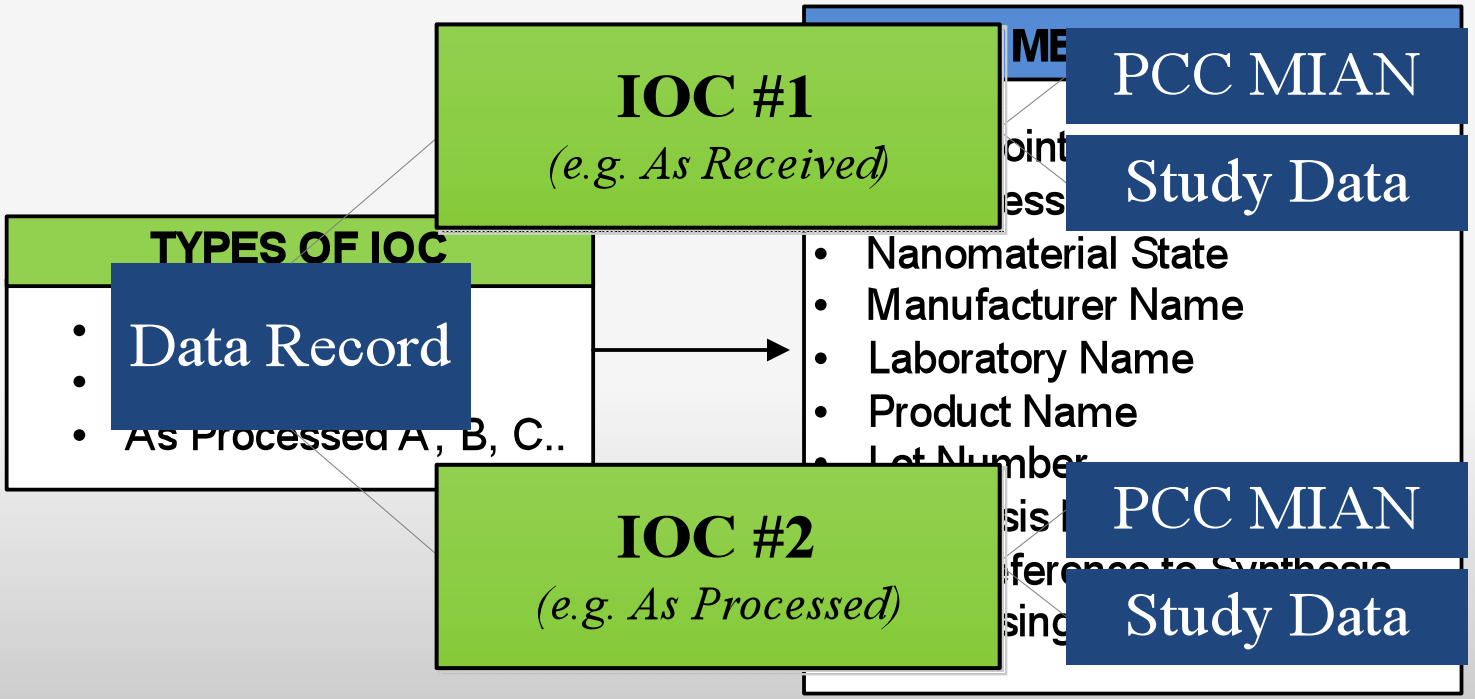
DATA INSTANCE OF CHARACTERIZATION



NANOMATERIALREGISTRY

DATA RECORD

NM CHARACTERIZATION *Example Record: NR1130*

- ✓ Composition
- ✓ Size
- Size Distribution
- ✓ Shape
- Aggregation/Agglomeration State
- Surface Area
- ✓ Surface Charge
- Surface Chemistry
- Surface Reactivity
- Purity
- Solubility
- Stability

MIAN PCC Information from NR1130:

Material Type: **Metal** Molecular Identity: **Silver**	IOC = As Sythesized
Primary Particle Size: **10 nm** Core Size: **5 nm (Gold Core)**	
Mean Hydrodynamic Diameter: **21.7 ± 0.3 nm** *Dynamic Light Scattering*	IOC = As Processed A suspended in water (for DLS)
Zeta Potential: **-40.6 ± 0.4 mV** *Electrophoretic Light Scattering*	
Mean Diameter: **7.2 ± 1.2 nm** *Transmission Electron Microscopy*	IOC = As Processed B Dried (for TEM)
Dimensions in the Nanoscale: **3D** *Transmission Electron Microscopy*	

TYPES OF CHARACTERIZATION

MEASUREMENT VALUES & TECHNIQUES

ENVIRONMENTS & TIME POINTS

LOOKING ACROSS TECHNIQUES

Particle size is frequently reported **without technique**

(LOW DATA QUALITY RATING)

Dynamic light scattering is the most curated technique

Techniques used to measure particle size

LOOKING ACROSS PARAMETERS

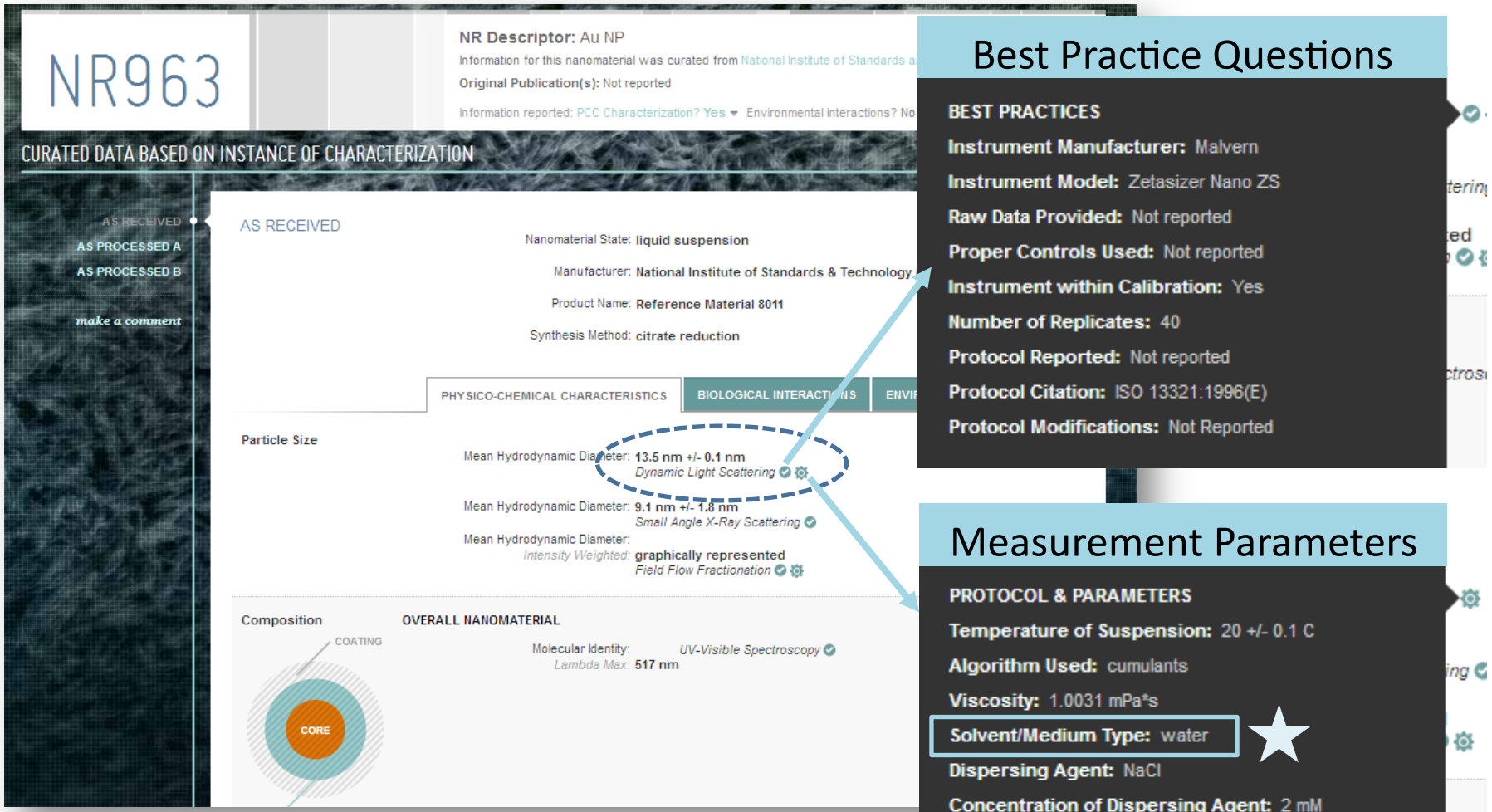
Solvent Type is the most frequently reported parameter for DLS

Other DLS parameters that are collected, but not shown here, include

- ✓ **scattering angle**
- ✓ **wave length**
- ✓ **index of refraction**

Parameters reported for Dynamic Light Scattering

DETAILS PAGE META DATA



Best Practice Questions

BEST PRACTICES

Instrument Manufacturer: Malvern
Instrument Model: Zetasizer Nano ZS
Raw Data Provided: Not reported
Proper Controls Used: Not reported
Instrument within Calibration: Yes
Number of Replicates: 40
Protocol Reported: Not reported
Protocol Citation: ISO 13321:1996(E)
Protocol Modifications: Not Reported

Measurement Parameters

PROTOCOL & PARAMETERS

Temperature of Suspension: 20 +/- 0.1 C
Algorithm Used: cumulants
Viscosity: 1.0031 mPa*s
Solvent/Medium Type: water
Dispersing Agent: NaCl
Concentration of Dispersing Agent: 2 mM
Sample Concentration: diluted 6-fold
Sonication/Milling Power: none
Sonication/Milling Time: none

NIST Reference Material 8011 – Citrate stabilized Au NP

NANOMATERIALREGISTRY

Compliance Levels in the Nanomaterial Registry

DATA QUALITY

DATA QUALITY METRIC

The Nanomaterial Registry's **COMPLIANCE LEVEL FEATURE** provides a **METRIC** on the **QUALITY** of characterization of a nanomaterial entry

Compliance Level	Score	Medal
Gold	76-100	
Silver	51-75	
Bronze	26-50	
Merit	0-25	

COMPLIANCE LEVELS are broken into **MERIT**, **BRONZE**, **SILVER**, and **GOLD** and represent increasing quality of characterization based on our evaluation criteria

A COMPLIANCE LEVEL SCORE is a quantitative value calculated by an algorithm

MORE INFORMATION: https://www.nanomaterialregistry.com/about/HowIsComplianceCalculated.aspx

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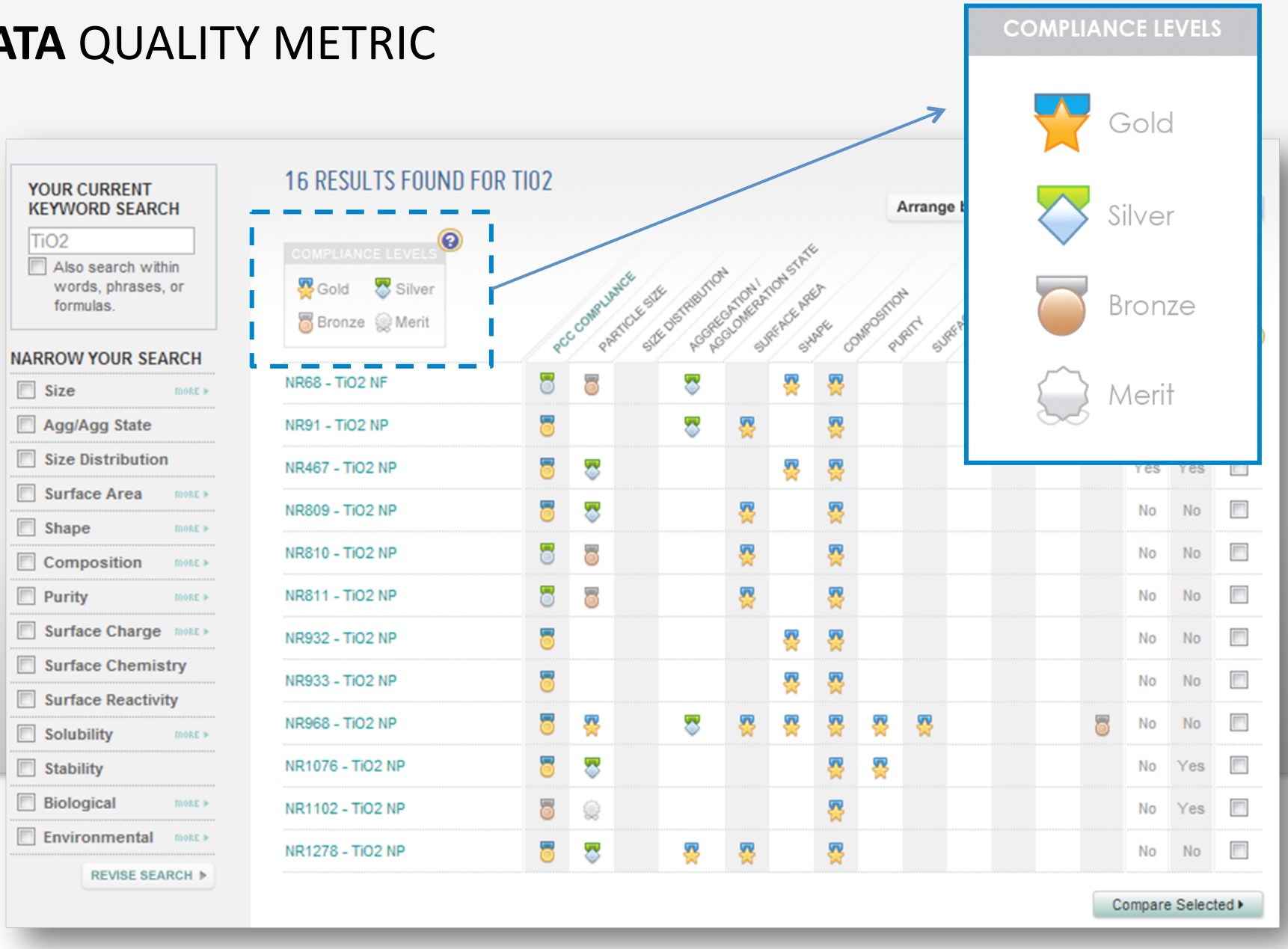
DATA QUALITY METRIC



www.nanomaterialregistry.org

DATA QUALITY METRIC

Records with more specific measurement data are awarded more points than those with less specific data

Scenario 1	Scenario 2	Scenario 2	Scenario 4
Size= 37.5 nm	***Size= 37.5 nm*** **Mean Hydrodynamic Diameter**	***Size= 37.5 nm*** ***Mean Hydrodynamic Diameter*** **Dynamic Light Scattering** **Malvern ZetaSizer Nano ZS**	***Size= 37.5 nm*** ***Mean Hydrodynamic Diameter*** ***Dynamic Light Scattering*** ***Malvern ZetaSizer Nano ZS*** **11 of 12 measurement parameters reported** **Protocol: ASTM E2490 - 09**
Merit	**Bronze**	**Silver**	**Gold**

Algorithm

Assigns weights to each value that appears in a curated record

$$CL_{PCC} = \sum_{Measurements} \left\{ \frac{\sum_G M_G * P_G}{\sum_G M_G * W_G} \right\}$$

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NANOMATERIALREGISTRY

THANK YOU!

www.nanomaterialregistry.org

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